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HOST-GUEST INTERACTIONS BETWEEN NIOBIUM POLYOXOMETALATES AND NEUTRAL AZA-MACROCYCLES

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During recent semesters, Dr. Roesner's research group has been investigating interactions between aza-macrocycles and polyoxometalates with the long-term goal of using polyoxometalates to direct the assembly of those macrocycles into supramolecular species. During those initial investigations, the group focused on Keggin polyoxoanions (e.g. $PW_{12}O_4^{3^-}$, $SiW_{12}O_4^{4^-}$), which are stable only at low pH conditions that also lead to protonation of the aza-macrocycles. The resulting polyoxoanion/ macrocycle adducts had properties consistent with the strong ionic bonds that held them together. They were poorly soluble in both water and polar organic solvents. In an effort to develop more-soluble polyoxoanion/adducts, the synthesis of niobium polyoxometalates (e.g. $Nb_6O_{19}^{7^-}$ and $Nb_6O_{19}^{6^-}$) is now underway. These niobium polyoxometalates are stable in basic solution where it will be possible to observe their interactions with neutral (free base) aza-macrocycles. It is hoped that the weaker, ion-dipole forces present in these systems will allow for greater solubility. This solubility should, in turn, allow for more-thorough spectroscopic investigation and the possibility of carrying out solution-based organic transformations on the polyoxoanion/macrocycle adducts.